

Quantum critical phase diagram of bond alternating Ising model with Dzyaloshinskii-Moriya interaction: signature of ground state fidelity

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We present the zero temperature phase diagram of the bond alternating Ising chain in the presence of Dzyaloshinskii-Moriya interaction. An abrupt change in ground state fidelity is a signature of quantum phase transition. We obtain the renormalization of fidelity in terms of quantum renormalization group without the need to know the ground state. We calculate the fidelity susceptibility and its scaling behavior close to quantum critical point (QCP) to find the critical exponent which governs the divergence of correlation length. The model consists of a long range antiferromagnetic order with nonzero staggered magnetization which is separated from a helical ordered phase at QCP. Our results state that the critical exponent is independent of the bond alternation parameter (λ) while the maximum attainable helical order depends on λ .

I. INTRODUCTION

One of the key features of strongly correlated electron systems is their zero temperature behavior where quantum fluctuations have the dominant role to classify different novel phases which are separated by quantum phase transitions¹. In this case, ground state (GS) is the sole candidate which receives drastic changes at QCP driven by some external parameters. Identification of QCPs is always a challenging task specially when quantum correlations diminish a single-particle picture. Within last couple of years different measures of quantum entanglement have been proposed to be a new toolkit to detect and categorize QCPs². Recently, ground state fidelity—the overlap of ground state at two slightly different values of coupling constants—has attracted intensive attention as a proper quantity to signal QCP without the need to know the structure of phases close to phase transition^{3,4}.

An abrupt drop of fidelity in the vicinity of QCP is a consequence of an essential change in the structure of GS which is usually accompanied with a divergence of fidelity susceptibility. Meanwhile, it is rather difficult to obtain the GS of a strongly correlated many body system. However, recent successful attempts to calculate some measures of entanglement⁵ by quantum renormalization group (QRG) approach⁶ lead to a unified formalism⁷ to obtain fidelity in the thermodynamic limit ($N \rightarrow \infty$) without knowing the GS of a large system. It suggests to implement QRG for obtaining the renormalization of fidelity for the bond alternating Ising model with Dzyaloshinskii-Moriya (DM) interaction. DM interaction^{8,9} which roots to the spin-orbit coupling is the antisymmetric super-exchange which leads to helical magnetic structures as the most likely candidates to host ferroelectricity¹⁰.

In this article we study the quantum critical behavior of the one dimensional bond alternating Ising model with DM interaction in terms of renormalization of fidelity. The model represents an antiferromagnetic (Néel) long range order for small DM interaction while it undergoes via a continuous phase transition to a helical ordered phase. The ground state in the Néel phase is a product state which has essentially zero quantum entanglement and nonzero staggered magnetization while the helical phase poses a correlated quantum ground

state with zero staggered magnetization. Within a classical picture the helical phase could be assumed as slightly rotating spins along the direction of chain. In terms of Landau theory of critical phenomena the staggered magnetization could be chosen as the proper order parameter. We have shown that the divergence in fidelity susceptibility (FS) at the QCP is an appropriate signature to find QCP which is more pronounced than the second derivative of ground state energy¹¹. The presented scheme makes us to find the critical points and its corresponding exponents more accurately.

II. QUANTUM RENORMALIZATION GROUP

The Hamiltonian of bond alternating Ising chain with DM interaction on a periodic chain of N sites is defined

$$H = J \sum_{i=1}^N \left[(1 - (-1)^i \lambda) S_i^z S_{i+1}^z + \vec{D} \cdot (\vec{S}_i \times \vec{S}_{i+1}) \right], \quad (1)$$

where \vec{S}_i is the spin-1/2 operator at site i , λ describes the relative strength of the alternating coupling and $J > 0$ shows the nearest-neighboring antiferromagnetic coupling. \vec{D} is the vector of DM interaction which is considered in z -direction, i.e. $\vec{D} = D \hat{z}$. To apply QRG⁶, the spin chain is decomposed to three-sites blocks (see Fig.1) where the intra-block Hamiltonian is H^B and the inter-block one is H^{BB} and their sum defines the whole Hamiltonian, $H = H^B + H^{BB}$ (see the bottom part of Fig.1). In this respect we have $H^B = \sum_{I=1}^{N/3} h_I^B$, where

$$h_I^B = J \sum_{l=1}^2 \left([1 + (-1)^{I+l} \lambda] S_{l,I}^z S_{l+1,I}^z + D(S_{l,I}^x S_{l+1,I}^y - S_{l,I}^y S_{l+1,I}^x) \right), \quad (2)$$

and similarly $H^{BB} = \sum_{I=1}^{N/3} h_{I,I+1}^{BB}$,

$$h_{I,I+1}^{BB} = J \left([1 - (-1)^I \lambda] S_{3,I}^z S_{1,I+1}^z + D(S_{3,I}^x S_{1,I+1}^y - S_{3,I}^y S_{1,I+1}^x) \right). \quad (3)$$

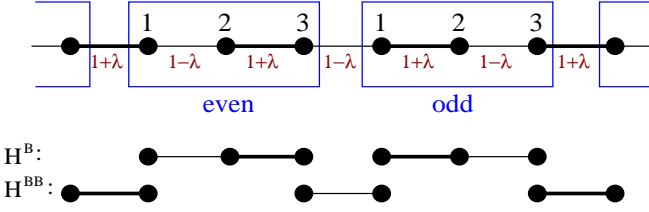


FIG. 1. Decomposition of the lattice to 3-sites blocks. The intra-block Hamiltonian (H^B) and inter-block one (H^{BB}) are represented schematically in the bottom part.

The block Hamiltonian (h_I^B) is diagonalized exactly and the two lowest energy eigenvectors ($|\Psi_I^\pm\rangle$) are kept to construct the embedding operator (P_I) to the renormalized Hilbert space, $P_I = |\Psi_I^+\rangle\langle\uparrow\uparrow| + |\Psi_I^-\rangle\langle\downarrow\downarrow|$. Here, $|\uparrow\rangle, |\downarrow\rangle$ represent the renamed states $|\Psi_I^+\rangle$ and $|\Psi_I^-\rangle$, respectively in the renormalized space to be considered as the new base kets. $|\Psi_I^+\rangle$ and $|\Psi_I^-\rangle$ have the following expression (for odd blocks) in the original spin Hilbert space where $|\uparrow\rangle$ and $|\downarrow\rangle$ represent the eigenvectors of S^z operator at each site,

$$\begin{aligned} |\Psi_I^+\rangle &= a|\uparrow\uparrow\downarrow\rangle + ib|\uparrow\downarrow\uparrow\rangle + c|\downarrow\uparrow\uparrow\rangle, \\ |\Psi_I^-\rangle &= a|\downarrow\downarrow\uparrow\rangle - ib|\downarrow\uparrow\downarrow\rangle + c|\uparrow\downarrow\downarrow\rangle, \end{aligned} \quad (4)$$

where

$$a = \frac{bD}{(\lambda - 2\varepsilon_0)}, b = \frac{1}{\sqrt{1 + \frac{2D^2(4\varepsilon_0^2 + \lambda^2)}{(4\varepsilon_0^2 - \lambda^2)^2}}}, c = \frac{bD}{(\lambda + 2\varepsilon_0)}, \quad (5)$$

and ε_0 is the ground state energy of the block. The presence of bond alternation imposes to consider two types of blocks as depicted in Fig.1, namely even and odd which are the mirror image of each other. For even blocks we find similar eigenstates by replacing $a \rightarrow -c$, $b \rightarrow b$ and $c \rightarrow -a$.

The global embedding operator is the direct product of the embedding operator of each block, $P = \otimes_I^{N/3} P_I$ which gives the renormalized Hamiltonian by $H^{ren} = P^\dagger H P$. The renormalized Hamiltonian is similar to the original one, Eq.1, while the coupling constants are replaced with the renormalized one (denoted with $'$) as given in the following equations,

$$J' = XJ, \quad \lambda' = \lambda, \quad D' = -\frac{4ab^2c}{X}D, \quad (6)$$

where $X = (1 - 2a^2)(1 - 2c^2)$. These relations, Eq.6, define the QRG-flow of our model which will be used in next sections and their features will be discussed in Sec.III.

A. Fidelity signature

We implement the formalism introduced in⁷ to calculate the ground state fidelity in terms of quantum renormalization group. According to the QRG-flow (Eq.6), λ does not run

within the QRG iterations which hints to study the quantum phase transition by variation of D . The fidelity (f) associated to the ground states $|\Psi(D)\rangle$ for a system of size N is defined by

$$f(D, \delta; N) = \langle \Psi(D_-) | \Psi(D_+) \rangle, \quad (7)$$

where $D_\pm = D \pm \delta/2$ and δ is a small deviation around D . According to the renormalization group approach $|\Psi\rangle = P|\Psi^{(1)}\rangle$ in which P is the global embedding operator and $|\Psi^{(1)}\rangle$ is the ground state of the renormalized Hamiltonian. Thus, fidelity can be written in terms of renormalized ground state, $f = \langle \Psi^{(1)}(D_-) | P^\dagger(D_-) P(D_+) | \Psi^{(1)}(D_+) \rangle$. A straightforward calculation shows that

$$\begin{aligned} P_I^\dagger(D_-) P_I(D_+) &= R_0(D_-, D_+) \mathcal{I}, \\ R_0 &= [a(D_-)a(D_+) + b(D_-)b(D_+) + c(D_-)c(D_+)], \end{aligned} \quad (8)$$

for both even and odd types of blocks where \mathcal{I} is the identity operator. Therefore, the first QRG iteration leads to $f = R_0^{\frac{N}{3}}(D_-, D_+) \times \langle \Psi^{(1)}(D_-) | \Psi^{(1)}(D_+) \rangle$, where fidelity of the original model is expressed in terms of fidelity of the renormalized one, i.e. $f = R_0^{\frac{N}{3}} f^{(1)}$. It defines the renormalization of fidelity in terms of QRG. The QRG procedure is iterated n -times to reach the renormalized system of $N = 3^{n+1}$ and the ground state fidelity is expressed by

$$f = \left(\prod_{i=0}^{n-1} R_i^{\frac{N}{3^{i+1}}} \right) \langle \Psi^{(n)}(D_-) | \Psi^{(n)}(D_+) \rangle, \quad (9)$$

where R_i has the same expression as given in Eq.8 for R_0 in which a , b and c are calculated at the i -th QRG iteration and $\langle \Psi^{(n)}(D_-) | \Psi^{(n)}(D_+) \rangle$ is the fidelity of a single block with three sites and n -times renormalized couplings.

We have plotted fidelity (Eq.9) versus D in Fig.2-(left) for different chain length (N), $\delta = 0.01$ and at $\lambda = 0.5$. By definition, fidelity is bounded by $0 \leq f \leq 1$ and an abrupt drop is a signature of quantum phase transition. We observe a sharp drop in Fig.2-(left) for $0.8 < D < 0.9$ which manifests that the ground state has encountered an essential change. The deep of drop is enhanced as the system size is increased which justifies an unfailing drop in the thermodynamic limit. This signature of quantum phase transition is more pronounced in the fidelity susceptibility (FS) which is the leading nonzero term in the expansion of fidelity and shows the change rate of fidelity, i.e. $f = 1 - \frac{\delta^2}{2} FS + O(\delta^3)$. Thus, FS is obtained by the following relation

$$FS = \lim_{\delta \rightarrow 0} 2 \frac{1-f}{\delta^2}. \quad (10)$$

Fig.2-(right) presents FS versus D for various system sizes, $\delta = 0.01$ and at $\lambda = 0.5$. A maximum appears in $D = D_{max}(N)$ which is increased by the size of system representing a divergence in the thermodynamic limit. The position of $D_{max}(N)$ is exactly at the point where fidelity receives a drop.

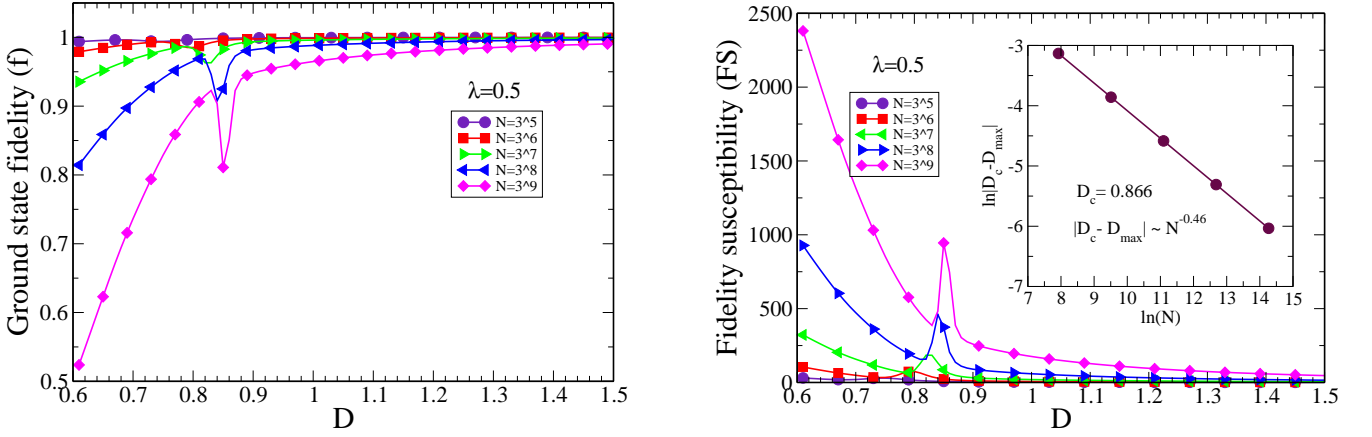


FIG. 2. (Left) Ground state fidelity (f) versus Dzyaloshinskii-Moriya interaction strength (D) for different chain size and at $\lambda = 0.5$. (Right) Fidelity susceptibility (FS) versus D at $\lambda = 0.5$ for various system sizes $N = 3^5, \dots, 3^9$. Inset: the scaling behavior shows how the maximum of FS (D_{max}) approaches the critical point (D_c) by increasing size. In both figures $\delta = 0.01$ which is the difference between two parameters ($D_+ - D_- = \delta$) to calculate fidelity in the left figure and according to Eq.(10) for the right figure.

B. Scaling analysis

It has been shown⁴ that the fidelity susceptibility at the quantum critical point obeys a scaling relation. The scaling analysis for finite system size (N) states

$$|D_c - D_{max}| \sim N^{-\frac{1}{\nu}}, \quad (11)$$

where D_c is the quantum critical point, D_{max} is the position of maximum in FS and ν is the critical exponent governing the divergence of correlation length. The analysis of data of Fig.2-(right) is presented as an inset to this figure. It clearly verifies that the scaling relation Eq.11 is satisfied with $D_c \simeq 0.866$ and $\nu \simeq 2.17$ for $\lambda = 0.5$. Moreover, we have obtained similar behavior for different values of λ (not presented here) where the critical point is found to be a function of bond alternating parameter, $D_c \simeq \sqrt{1 - \lambda^2}$ while $\nu \simeq 2.17$ is the same for all values of λ . In contrast to what stated in Ref.¹² the critical exponent which we got does not depend on λ . It means that the whole phase boundary for $0 \leq \lambda < 1$ belongs to the same universality class of a second order phase transition.

III. SUMMARY AND DISCUSSIONS

We have implemented the quantum renormalization group approach to study the zero temperature phase diagram of bond alternating Ising chain in the presence of DM interaction. To get a self similar Hamiltonian two types of blocks with 3-sites have been considered which leads to the QRG-flow equations of Eq.6. The QRG-flow tells that λ does not vary within QRG procedure while D is renormalized. To get the phase diagram of the model we have calculated the renormalization of ground state fidelity which has been developed recently⁷.

Fidelity as a geometric quantity¹⁴ shows how much the ground state encounters an essential change by slightly moving in the parameter space. Therefore, a sharp drop of fidelity versus a control parameter is a signature of quantum phase transition. The renormalization of fidelity obtained in Eq.9 in addition to QRG-flow, Eq.6 give the fidelity of our model for very large system sizes without the need to get the ground state. A clear drop of fidelity versus D in Fig.2-(left) and consequently a maximum in the fidelity susceptibility, Fig.2-(right), verifies the existence of a quantum phase transition at D_c . We have applied the finite size scaling on the susceptibility data presented in the inset of Fig.2-(right) for $\lambda = 0.5$ and generally got the critical phase boundary $D_c \simeq \sqrt{1 - \lambda^2}$. The phase boundary which separates the antiferromagnetic (AF) Néel order from a helical order is shown by the blue line in Fig.3-(right). However, our scaling analysis gives a single value for the correlation length exponent $\nu \simeq 2.17$ (independent of λ) for the whole phase boundary which is in contrast to¹². Although the presence of bond alternation breaks the translation invariance of the Hamiltonian it does not change the symmetry of the ground state which has already been spontaneously broken due to antiferromagnetic long range order. A comparison of our results with¹³ concludes that the bond alternation does not change the universality class of the model as far as $\lambda \neq 1$.

We calculate the staggered magnetization (SM) and helical order parameter which is presented in Fig.3-(left). Staggered magnetization is defined by

$$SM = \frac{1}{N} \sum_{i=1}^N (-1)^i \langle \Psi | S_i^z | \Psi \rangle, \quad (12)$$

which can be expressed in terms of the renormalized ground state by replacing $|\Psi\rangle = P|\Psi^{(1)}\rangle$. We use the projection of spin operators into the renormalized Hilbert space which finally leads to

$$SM = -\frac{1 - 4b^2}{3} SM^{(1)}, \quad (13)$$

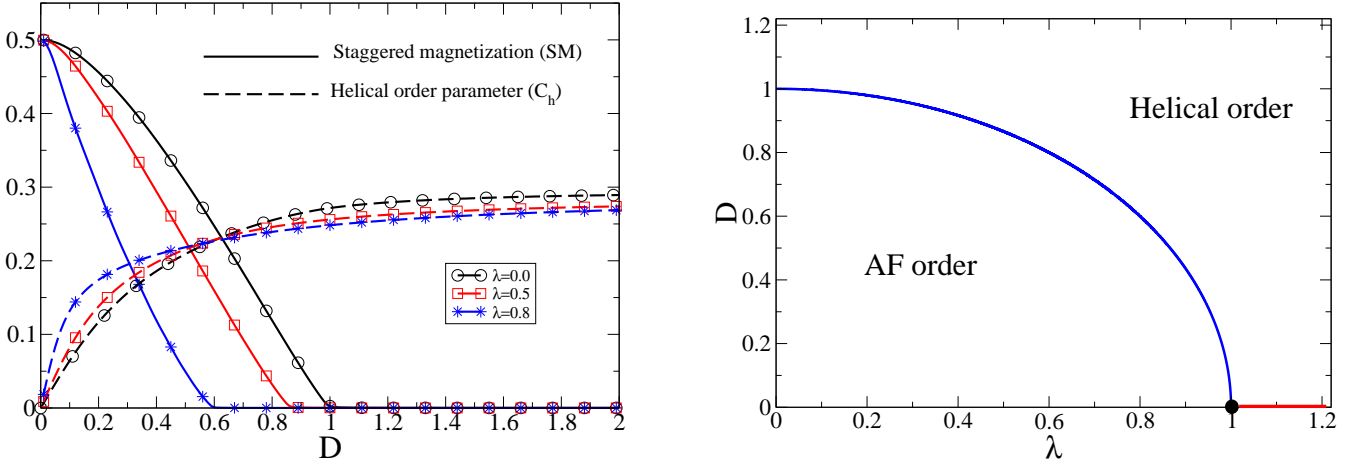


FIG. 3. (Left) Staggered magnetization (SM, solid lines) and helical order parameter (C_h , dashed lines) versus D for $\lambda = 0.0, 0.5, 0.8$. (Right) Zero temperature phase diagram in $\lambda - D$ plane. The blue curve represent the phase boundary between antiferromagnetic and helical ordered phases. The filled black circle denotes the first order tri-critical point and the red line shows a ferro-antiferromagnetic phase.

where $SM^{(1)}$ is the staggered magnetization of the renormalized chain. A large number of iterations of Eq.13 give the staggered magnetization in the thermodynamic limit. Similarly, the helical order parameter (C_h) is defined by the following relation¹³

$$C_h = \frac{1}{N} \sum_{i=1}^N \langle \Psi | (S_i^x S_{i+1}^y - S_i^y S_{i+1}^x) | \Psi \rangle, \quad (14)$$

which can be calculated using the QRG-flow. In this respect, C_h is expressed in terms of the helical order parameter in the renormalized model ($C_h^{(1)}$) by the following relation

$$C_h = C_h^{(0)} + \frac{\Gamma^{(0)}}{3} C_h^{(1)}, \quad (15)$$

$$C_h^{(0)} = \frac{b(a-c)}{3}, \quad \Gamma^{(0)} = -4ab^2c.$$

The above equation is iterated by replacing the couplings with the renormalized ones to reach the stable thermodynamic limit. We have plotted both staggered magnetization and helical order parameter versus D in Fig.3-(left) for three values of $\lambda = 0.0, 0.5, 0.8$ and $N \rightarrow \infty$. For $D = 0$, SM is at its saturated value 0.5 and $C_h = 0$. The onset of nonzero D induces a helical order on the spins in the presence of antiferromagnetic order. The increase of D reduces the antiferromagnetic order and enhances C_h (helical order). Exactly at the quantum critical point D_c , SM vanishes and remains zero for $D \geq D_c$ while C_h saturates to a finite amount which is less than its maximum attainable value. Similar behavior has been observed for all $0 \leq \lambda < 1$ while the saturated value of C_h is slightly decreased by increase of λ .

To complete the phase diagram let us concentrate on the $D = 0$ axis (Fig.3-(right)). At $\lambda = 0$ the model is simply an antiferromagnetic Ising chain with Néel order $|\uparrow\downarrow, \uparrow\downarrow$

, $\dots, \uparrow\downarrow\rangle$ and the ground state energy is $E_0 = -NJ/4$. For

$0 < \lambda < 1$, there are two types of couplings $(1 - \lambda)J$ and $(1 + \lambda)J$ which are positive and induce the previous Néel order and ground state energy. Exactly at $\lambda = 1$, the weak interaction $(1 - \lambda)J$ becomes zero and the spin model decomposes to $N/2$ independent pairs of antiferromagnetically coupled spins. The ground state energy is still $E_0 = -NJ/4$ while the ground state is exponentially degenerate, namely $2^{N/2}$. The degeneracy arises from the pairs which are decoupled. For instance, $|\uparrow\downarrow, \uparrow\downarrow, \dots, \uparrow\downarrow\rangle$, $|\downarrow\uparrow, \uparrow\downarrow, \dots, \uparrow\downarrow\rangle$ and $|\downarrow\uparrow, \downarrow\uparrow, \dots, \downarrow\uparrow\rangle$ are examples of different configurations which is possible for the ground state. The entropy (S) is proportional to $\ln(\text{\# of available states})$ which leads to $S \sim \ln(2^{N/2}) = \frac{N}{2} \ln 2$. This high amount of entropy at $\lambda = 1$ is a signature of a phase transition which is actually of first order. Meanwhile, for $\lambda > 1$ one of the interactions becomes ferromagnetic, $(1 - \lambda)J < 0$ and the other $(1 + \lambda)J$ is still antiferromagnetic which totally leads to $E_0 = -N\lambda J/4$. Thus, the derivative of E_0 with respect to λ receives a discontinuity at $\lambda = 1$. The ground state for $\lambda > 1$ is either $|\uparrow\downarrow, \uparrow\downarrow, \uparrow\downarrow, \uparrow\downarrow, \dots\rangle$ or $|\downarrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \uparrow\downarrow, \dots\rangle$. The first order tri-critical point is represented by the filled black circle in Fig.3-(right) and the ferro-antiferromagnetic ground state is denoted by the red line for $\lambda > 1$.

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